



Peridynamic Computational Model for Damage and Fracture

Stewart Silling
Paul Taylor

Dynamic Multiscale Material Modeling Department, 1435
Sandia National Laboratories

7th Biennial Tri-Laboratory Engineering Conference
May 9, 2007



Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company,
for the United States Department of Energy under contract DE-AC04-94AL85000.





Background: A better way to model cracks

- Problem
 - Develop a general tool for modeling material and structural failure due to cracks.
- Motivation
 - Fracture is a major mode of material failure.
 - Standard mathematical theory for modeling deformation cannot handle cracks.
 - PDE's break down if a crack is present.
 - Finite elements and similar methods inherit this problem.
- Approach
 - Develop a mathematical theory in which:
 - The same equations apply on or off of a crack.
 - Cracks are treated like any other type of deformation.
 - Cracks are self-guided: no need for supplemental equations.
 - Implement the theory in a meshless Lagrangian code called **EMU**.



Peridynamics – the basic idea

- PDEs are replaced by the following integral equation:

$$\rho \ddot{\mathbf{u}}(\mathbf{x}, t) = \int_H \mathbf{f}(\mathbf{u}' - \mathbf{u}, \mathbf{x}' - \mathbf{x}) dV - \mathbf{b}(\mathbf{x}, t) \quad (1)$$

- Compare classical PDE:

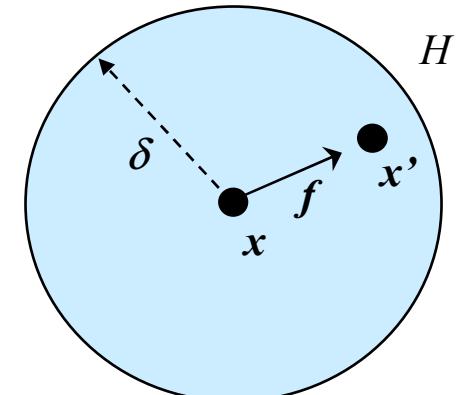
$$\rho \ddot{\mathbf{u}}(\mathbf{x}, t) = \nabla \bullet \boldsymbol{\sigma}(\mathbf{x}, t) - \mathbf{b}(\mathbf{x}, t) \quad (2)$$

where

\mathbf{u} = displacement; \mathbf{f} = force density that \mathbf{x}' exerts on \mathbf{x} ;

\mathbf{b} = prescribed external force density; H = neighborhood of \mathbf{x} with fixed radius δ ;

$\boldsymbol{\sigma}$ = stress tensor field.



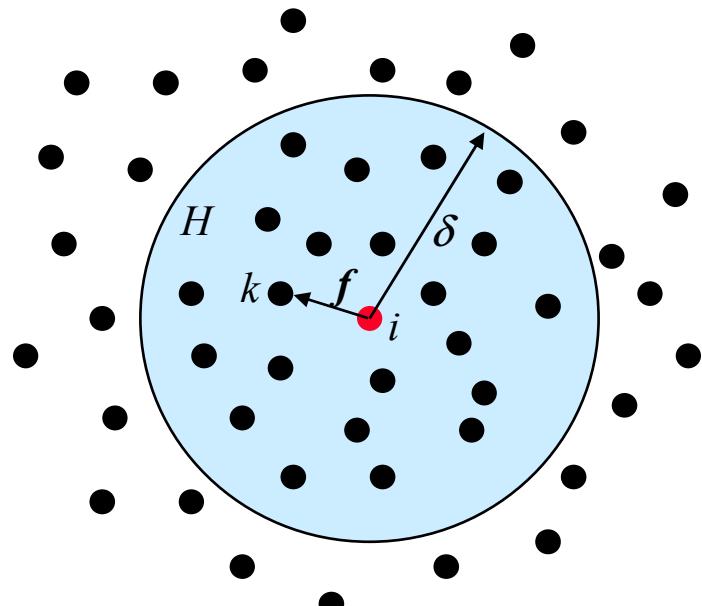
- New approach is more general than the classical model in the following ways:
 - (1) is not derivable from (2).
 - (1) converges to (2) in the limit $\delta \rightarrow 0$ (proof to be published).
 - (1) holds regardless of discontinuities.
 - (1) includes interaction between particles through a finite distance.
 - (1) is a “**Continuum version of molecular dynamics**”



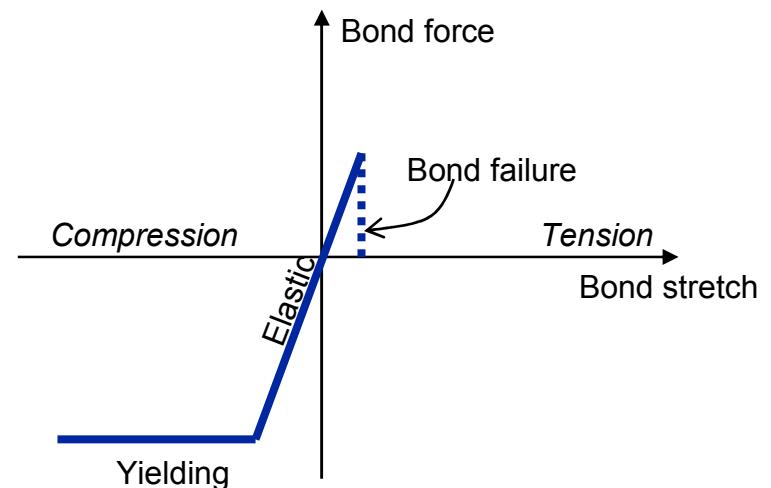
EMU numerical method and material model incorporate damage at the bond level

- Integral is replaced by a finite sum: resulting method is meshless and Lagrangian.
- Parameters come from measurable elastic-plastic and fracture data for materials.
- Sandia's Trilinos solver package is being applied to this method.

$$\rho \ddot{\mathbf{u}}_i^n = \sum_{k \in H} \mathbf{f}(\mathbf{u}_k^n - \mathbf{u}_i^n, \mathbf{x}_k - \mathbf{x}_i) \Delta V_i + \mathbf{b}(\mathbf{x}_i, t)$$



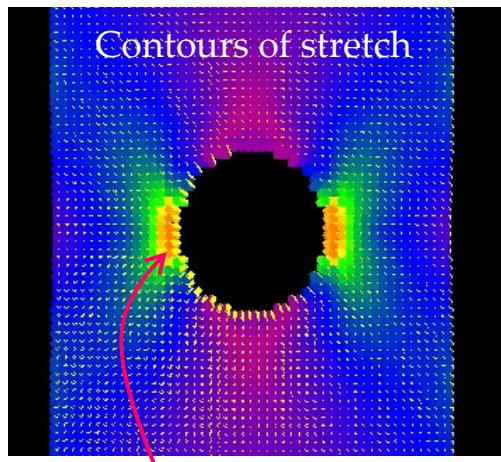
All material-specific behavior is contained in the function f .



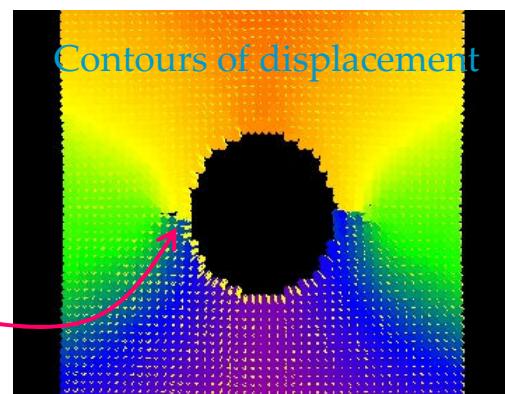


Initiation

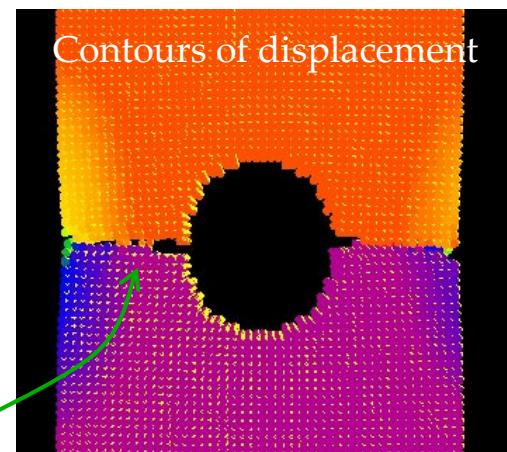
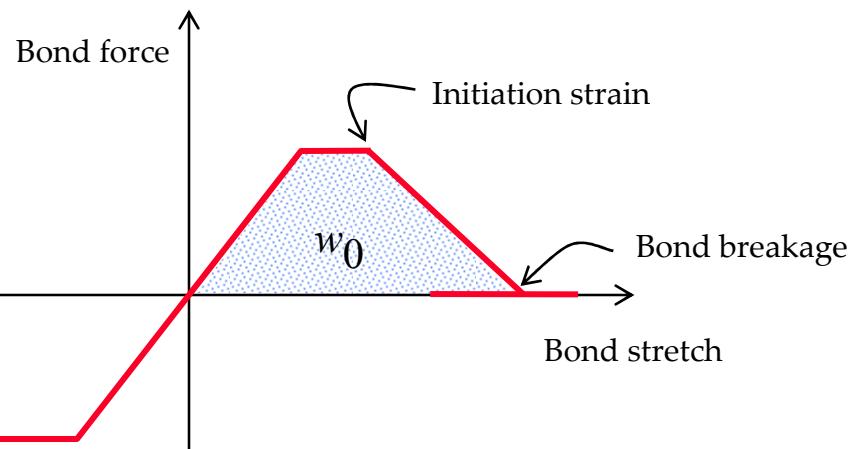
- A maximum in the bond force curve leads to crack initiation at a prescribed strain independent of the breakage stretch.



Stretch > initiation strain
leads to crack initiation

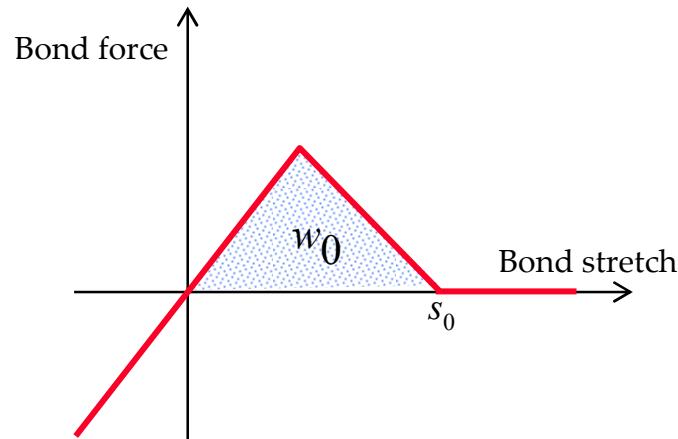


Crack initiation leads to
dynamic fracture



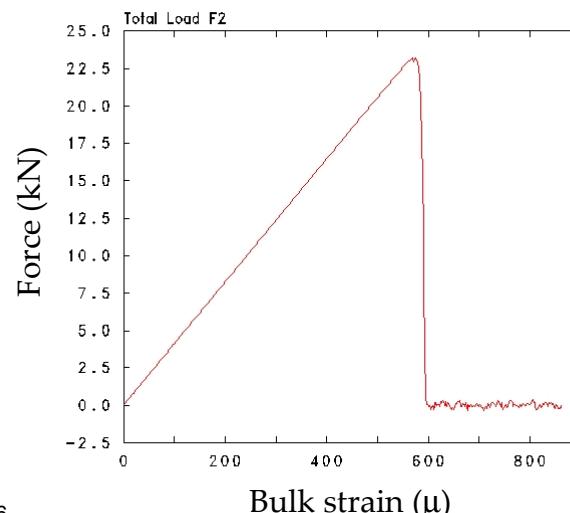
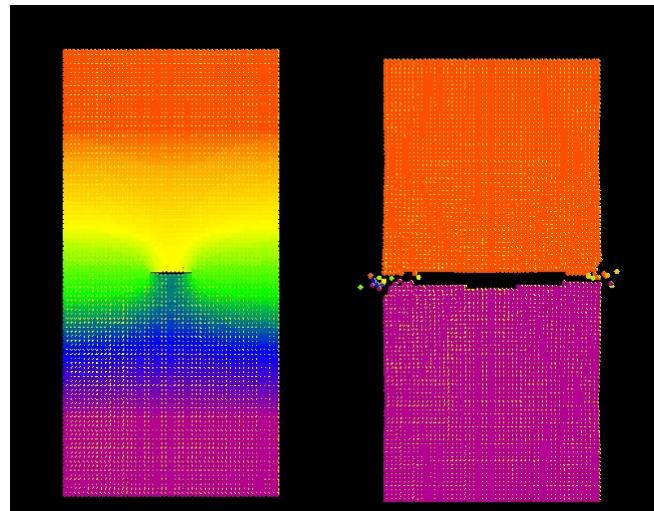


A validation problem: Center crack in a brittle panel (3D)



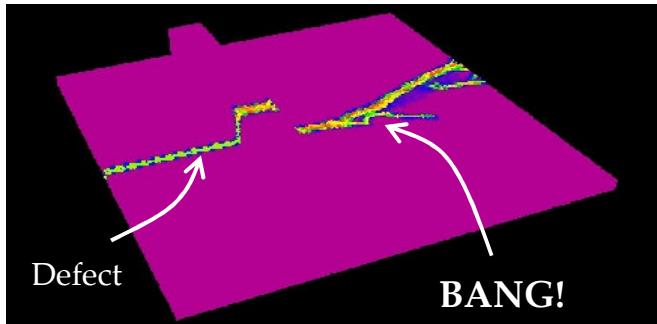
Based on $s_0=0.002$, find **$G=384 \text{ J/m}^2$** .
Full 3D calculation shows crack growth
when $\sigma=46.4 \text{ MPa}$. Use this in

$$G = \frac{\pi \sigma^2 a}{E} = 371 \text{ J/m}^2$$

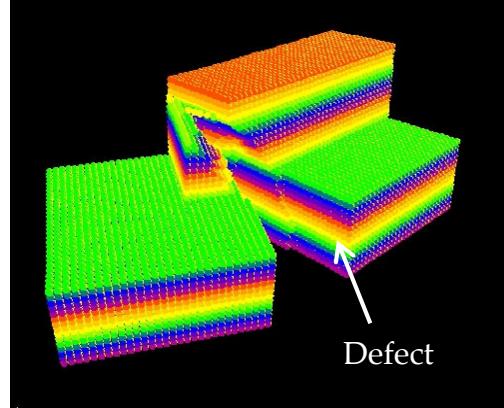




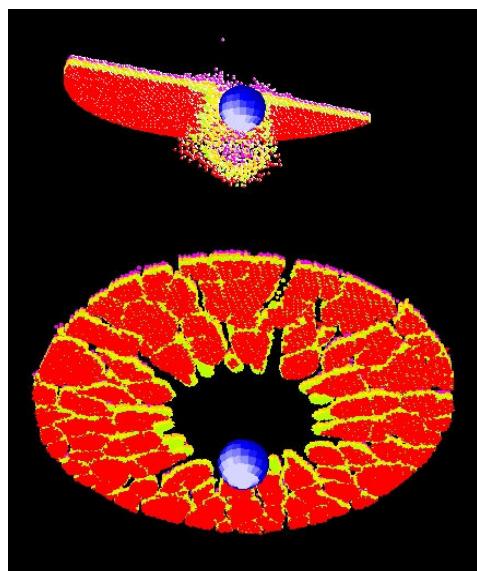
Isotropic materials: Other examples



Transition to unstable crack growth

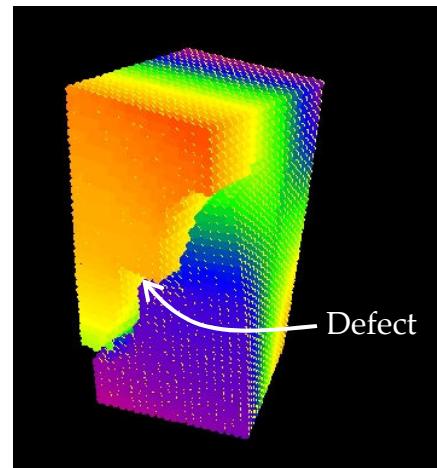


Crack turning in a 3D feature



Impact and fragmentation

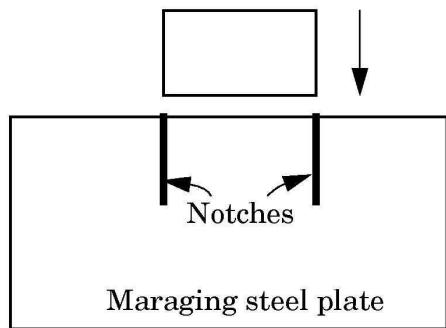
trilab_07_silling • frame 7



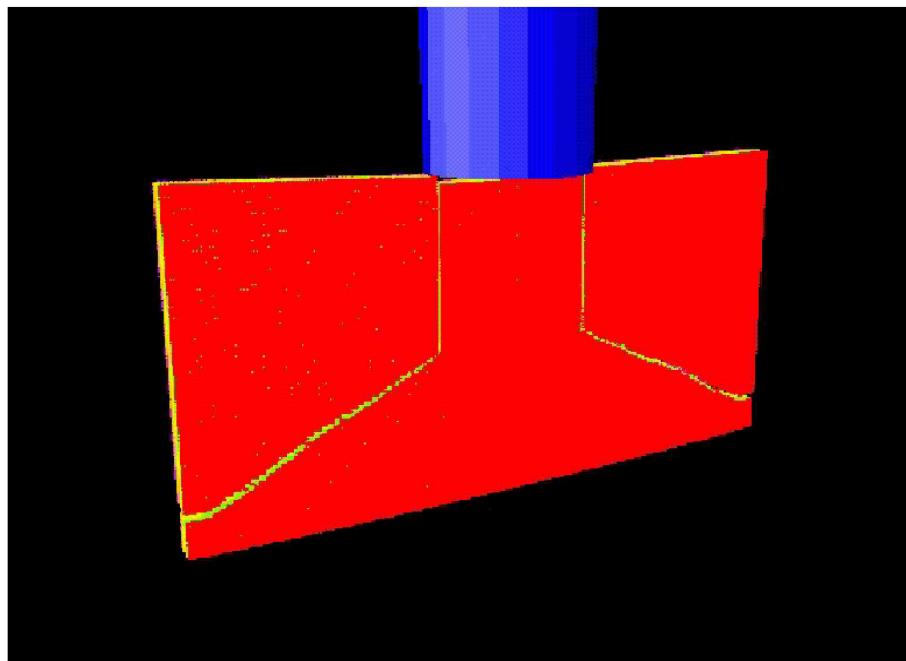
Spiral crack due to torsion



Example: dynamic fracture in steel



- Code predicts correct crack angles*.
- Crack velocity ~ 900 m/s.

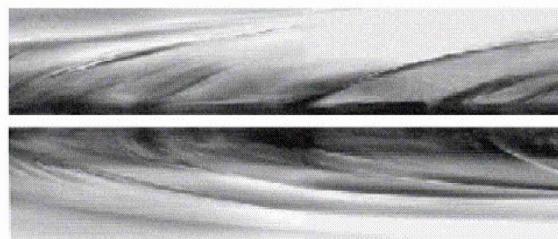
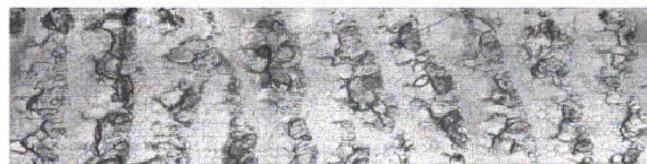
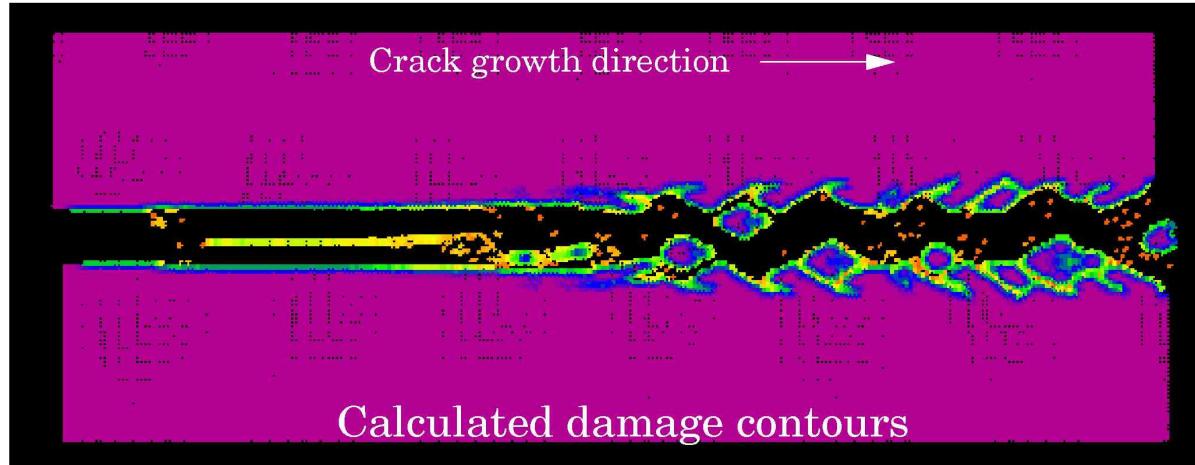


*J. F. Kalthoff & S. Winkler, in *Impact Loading and Dynamic Behavior of Materials*, C. Y. Chiem, ed. (1988)

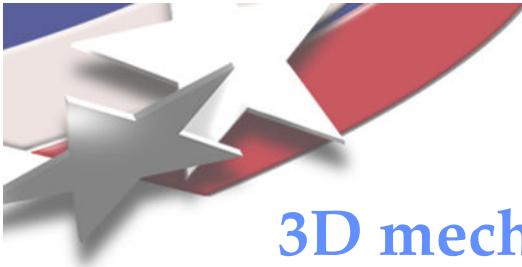


Example: dynamic fracture in PMMA

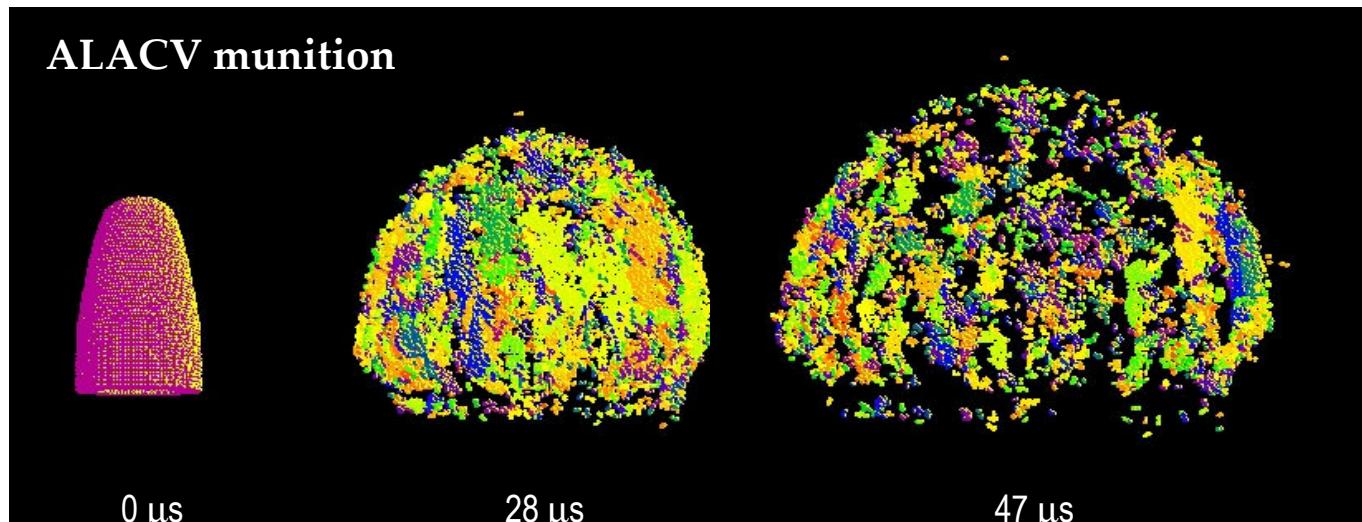
- Plate is stretched vertically.
- Code predicts stable-unstable transition.



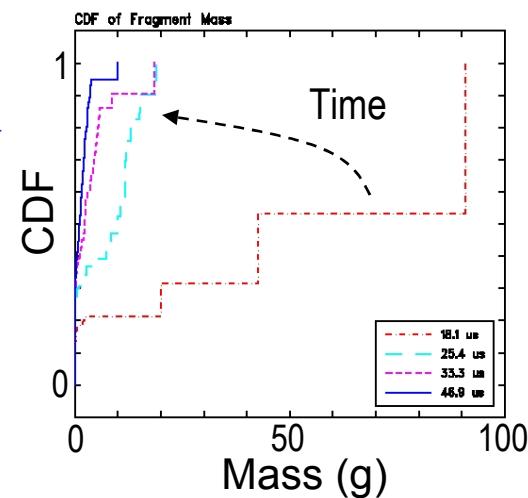
*J. Fineberg & M. Marder, *Physics Reports* **313** (1999) 1-108



Application (DoD/DOE MOU): 3D mechanics-based modeling of fragmentation



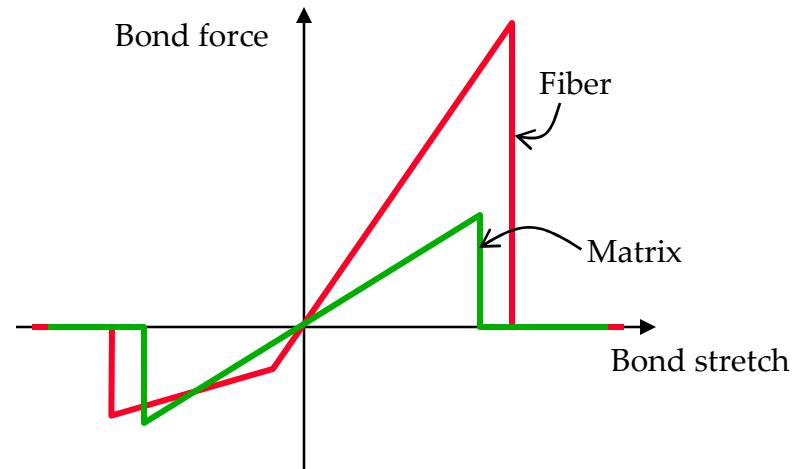
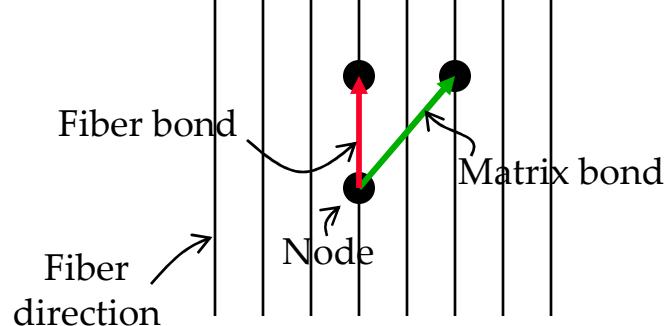
- CDF of fragment mass evolves over time.
- Method predicts statistical distribution of fragment energy, shape, and direction.
- Important application to NW safety.



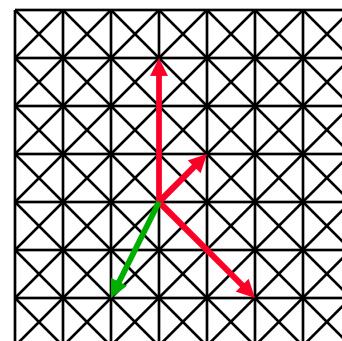


Composites: Peridynamic model of lamina

- Bonds parallel to fibers ($0^\circ, 45^\circ, \dots$) have special properties.



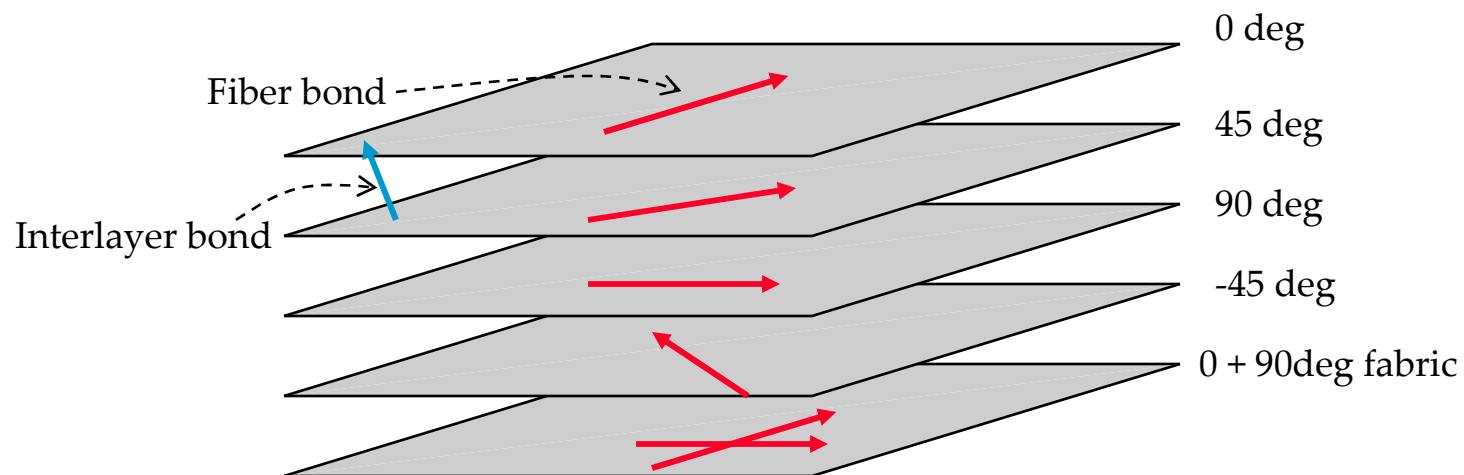
2D **laminate** model is just a lamina with fibers allowed in multiple directions (accounting for different fiber density in each direction)





3D peridynamic model of a laminate

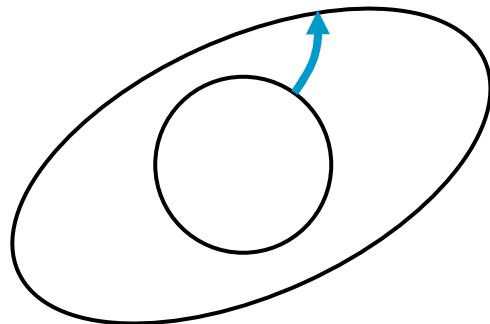
- Lamina models are stacked up according to the stacking sequence.
 - Lamina can contain multiple fiber directions (**fabric**).
 - Nodes in different lamina interact through **interlayer** peridynamic bonds.



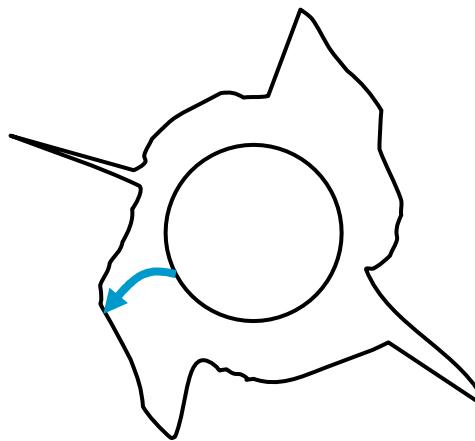


Peridynamic model of composites: Why take this approach?

- Classical ideas of stress and strain tensors break down in a damaged composite.
 - Traditional FE methods don't apply.
 - More “degrees of freedom” in a peridynamic deformation state allow for a greater range of failure phenomena to be captured.
 - Yet we can exploit traditional failure models if applicable.
- Natural correspondence between fibers and peridynamic bonds.
- Integral equations permit discontinuities in the mathematics.



Strain tensor maps any small sphere into some ellipsoid.

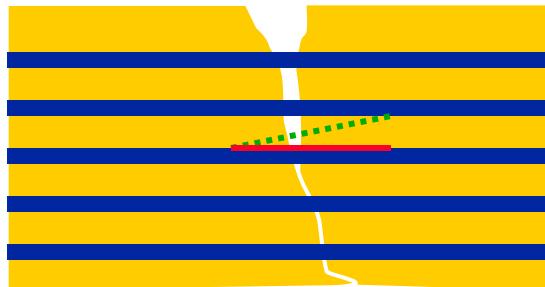


Peridynamic **deformation state** maps a sphere into whatever... “infinite degrees of freedom”

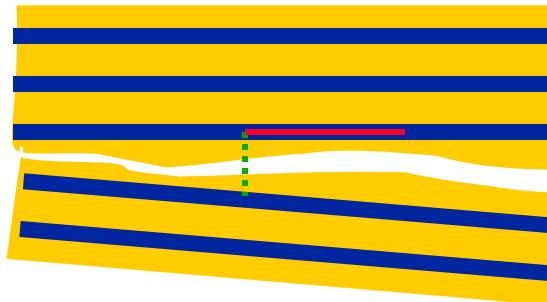


Peridynamic model of composites: Why take this approach?

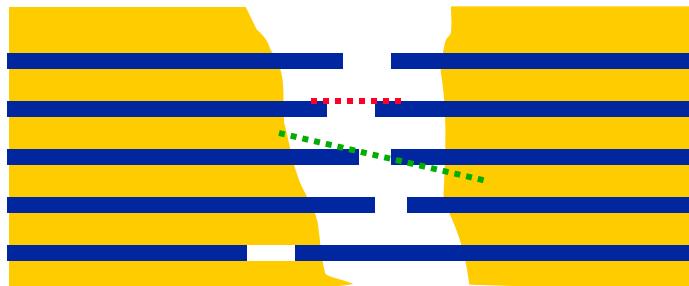
- Network of bonds gives a truer picture of failure modes.



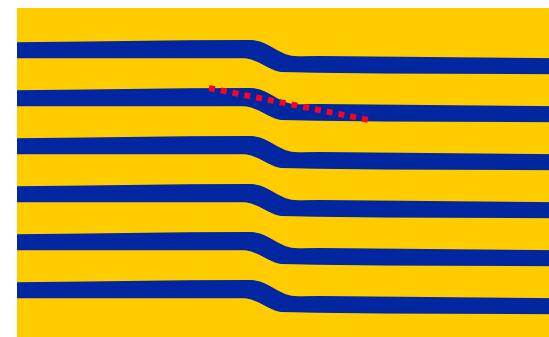
Bridging



Matrix cracking, debonding, delamination



Fiber tensile failure

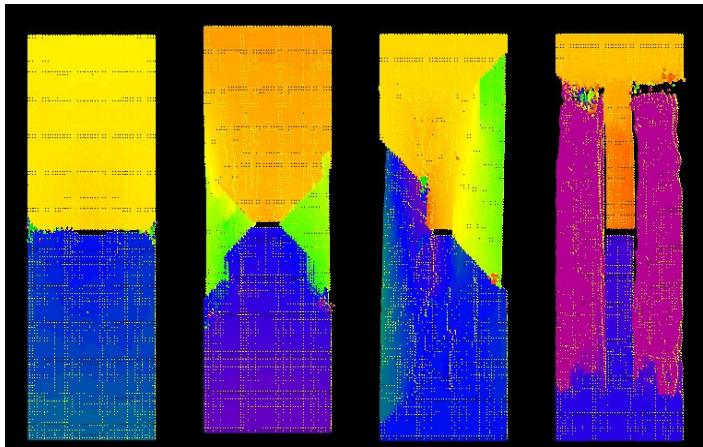


Fiber compressive failure

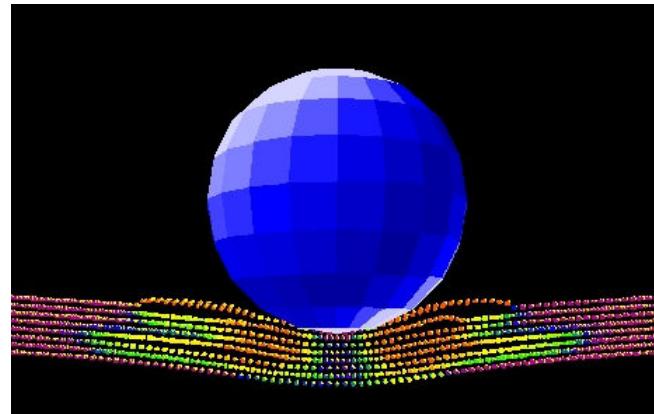


Composite material model applications

- How does the fraction of fibers in each direction affect the direction of crack growth?
- What damage occurs when a composite panel is struck by hail?



Crack growth in a notched panel

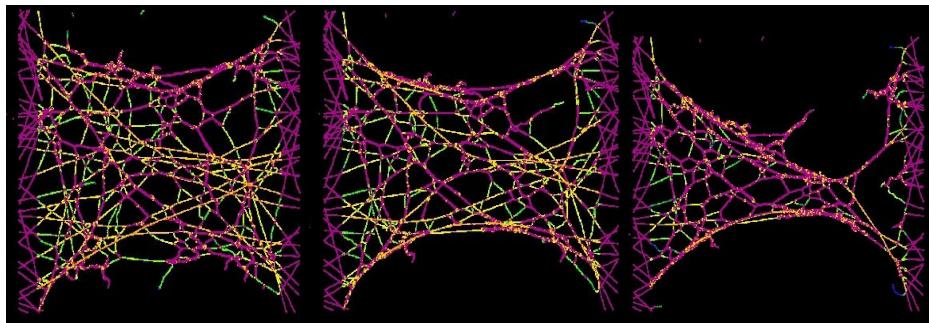


Delamination caused by impact

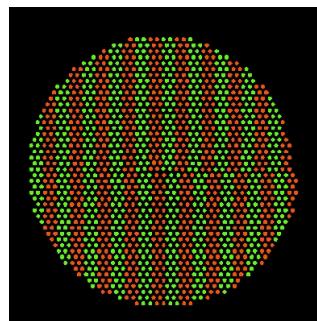


Nanoscale structural mechanics

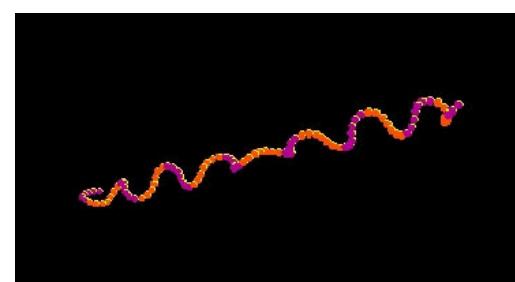
- Continuum version of molecular dynamics.
- All forces are treated as long-range.



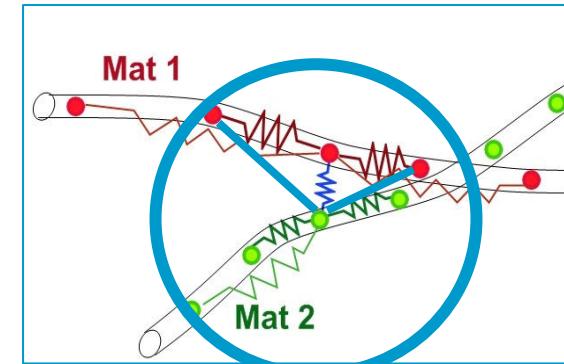
Failure in a nanofiber membrane
(F. Bobaru, Univ. of Nebraska)



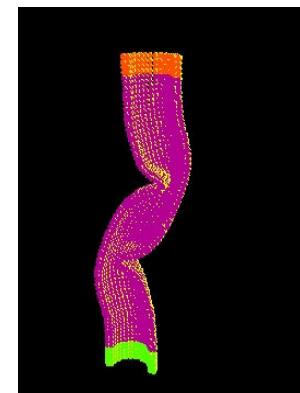
Dislocation



Nanofiber self-shaping



Nanofiber interactions due
to long-range forces



Carbon nanotube



Summary: Peridynamic vs. conventional model

- Theory
 - Different assumptions lead to different mathematics.
- Code
 - Discretized equations have different properties from finite elements.
 - Meshless, Lagrangian.
 - Easily implemented on parallel machines.
- Applications
 - New approach addresses the way materials **really** fail.
 - Method can incorporate nanoscale forces.
 - Length scale is variable – possible way to do multiscale modeling.